

Pyrogallol

87-66-1 | DTXSID6025983

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.81 | 0.55 | 0.81 | 0.54 | 0.71 | 0.61 |

Model Results

Predicted value: 38.4 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.89e-01

Confidence level: 8.07e-01

Nearest Neighbors from the Training Set

[Image not found](#)

1,2,3-Benzotriazole

Measured: 49.0

Predicted: 52.2

[Image not found](#)

Benzoic acid

Measured: 31.6

Predicted: 35.5

[Image not found](#)

Benzamide

Measured: 28.8

Predicted: 29.7

[Image not found](#)

6-Chloro-2-picolinic acid

Measured: 23.4

Predicted: 53.1